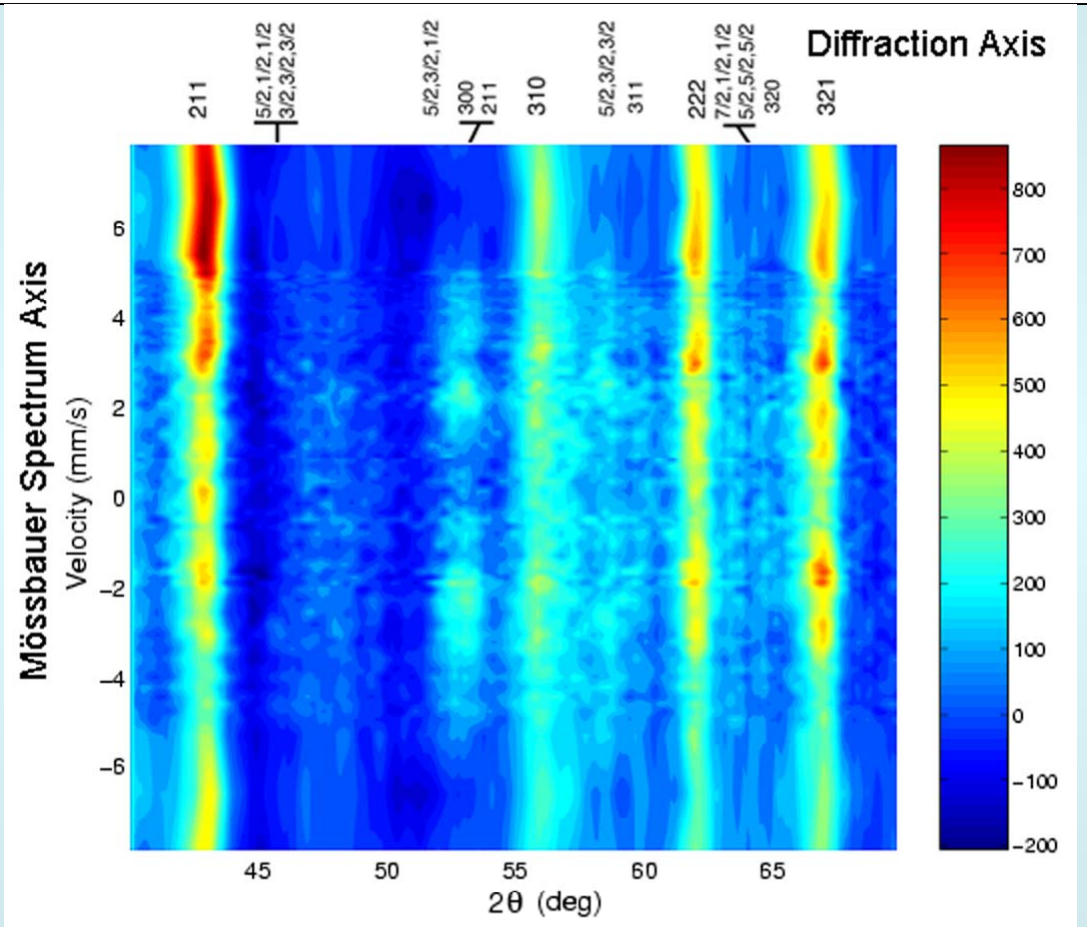
Mössbauer Diffractometry: A First Application to Materials Research

Brent Fultz, California Institute of Technology DMR-0204920

Mössbauer powder diffractometry combines the spatial information available from diffraction measurements with the chemical information available from spectrometry. The two axes of the experimental data show these two types of information.

The method was used for the first time in a study on real material to provide data on the long-range order of Fe atoms having different numbers of Al neighbors in Fe_3Al.

The measurements, with the support of simulations, showed that a significant fraction of Fe atoms with three Al 1nn are near antiphase domain boundaries.



Most of what we know about atomic arrangements in materials has been learned from diffraction experiments. To date, three scattering processes have proved useful for diffraction experiments: 1) scattering of x-rays by atomic electrons, 2) scattering of electrons from the electrons and nuclei of the atom, and 3) scattering of neutrons from nuclei or magnetic electrons. We built a powder diffractometer for Mössbauer diffraction, and have studied the method itself for several years. Mössbauer energy spectra, obtained from γ-ray scattering from nuclei, have been used widely for many years for identifying the different chemical environments of ^{57}Fe atoms in solids. We used the chemical environment selectivity of Mössbauer energy spectra to perform a new type of diffraction experiment — we tuned the incident photons so their diffraction patterns are modified by the chemical environments of the ^{57}Fe atoms.

In the first application of the method to a real problem in materials science, Mössbauer powder diffractometry was used recently to study partially-ordered Fe_3Al. Multiple diffraction patterns were measured at Doppler velocities across all nuclear resonances in the sample. The velocity-dependence of the superlattice diffractions (such as the (300) and (311) in the figure above) were analyzed, giving information on the long-range order of Fe atoms having different numbers of Al neighbors. Comparing experimental data to calculations showed that Fe atoms having three Al atoms as first-nearest neighbors (1nn) have simple cubic long-range order, similar to that of Fe atoms with four Al 1nn. The simple cubic periodicity of Fe atoms with three Al 1nn was significantly lower than expected for homogeneous antisite disorder, however. Monte--Carlo simulations and transmission electron microscopy suggest that a significant fraction of aperiodic Fe atoms with three Al 1nn are near antiphase domain boundaries.

J. Y. Y. Lin and B. Fultz, "Site-Specific Long-Range Order in $^{57}Fe_3Al$ Measured by Mössbauer Diffractometry", Philos. Mag. 83 (2003) 2621-2640.

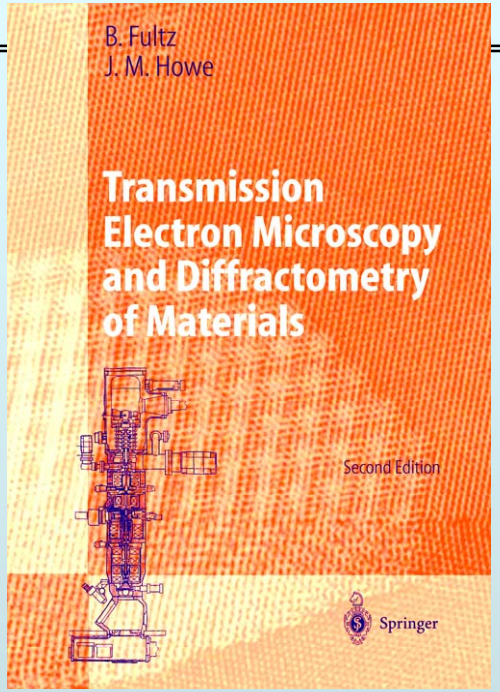
J. Y. Y. Lin and B. Fultz, “Mössbauer Diffractometry Measurements of Site-Specific Long-Range Order in $^{57}Fe_3Al$ ”, Zeitschrift fuer Kristallographie, 219 (2004) 172-178.

Mössbauer Diffractometry: A First Application to Materials Research

Brent Fultz, California Institute of Technology DMR-0204920

Broader Impact:

The concepts of diffraction and scattering developed under this program were important in setting the direction and style of the textbook *Transmission Electron Microscopy and Diffractometry of Materials*, B. Fultz and J. M. Howe, Springer-Verlag, now in its second edition.



Education:

Two graduate students contributed to this work:

Jiao Lin was awarded a Ph.D. from the California Institute of Technology for his dissertation supported under this award: *Mössbauer Diffractometry: Principles, Practice, and an Application to a Study of Chemical Order in* $^{57}Fe_3Al$.

Ryan Monson has begun work on his thesis research, with a focus on the development of high-performance solid-state detectors.